

# wwPDB EM Validation Summary Report (i)

#### Nov 20, 2022 – 12:35 AM EST

PDB ID	:	4V4W
EMDB ID	:	EMD-1143
Title	:	Structure of a SecM-stalled E. coli ribosome complex obtained by fitting atomic models for RNA and protein components into cryo-EM map EMD-1143
Authors	:	Mitra, K.; Frank, J.
Deposited on	:	2006-05-09
Resolution	:	15.00 Å(reported)
This is a	ww	PDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

:	0.0.1. dev 43
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.31.3
	: : : : :

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 15.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{f Entries})$		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		
RNA backbone	4643	859		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq=3, 2, 1$  and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq=5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length		Quality of chain	
			49%		
1	AA	1488	28%	53%	18% •
			46%		
2	AU	76	28%	58%	14%
			21%		
2	AV	76	30%	58%	12%
			30%		
2	AW	76	26%	59%	14%
				97%	
3	AB	236	44%	51%	•
				89%	
4	AC	206	40%	54%	5%
				99%	
5	AD	204	41%	57%	•



Mol	Chain	Length	Quality of chain							
6	AE	148	40%	86% 57%	<u> </u>					
				97%						
7	AF	95	33%	63%	•					
8	AG	137	49%	42%	9%					
0	A TT	197		100%						
9	Ап	127	40% 79	56% %	•					
10	AI	126	30%	61%	8% •					
11	AJ	96	34%	58%	7%					
12	AK	116	46%	47%	6% •					
13	AL	101	26%	49%	8%					
14	АМ	115	570/	33%	_					
	71111	110	57%	100%	•					
15	AN	61	44%	49%	7%					
16	AO	86	45%	55%						
17	AP	78	38%	56%	5%					
18	AQ	79	44%	9% 52%						
19	AR	69	42%	57%						
20		07		95%						
20	AS	01	37%	56%	7%					
21	AT	83	36%	55%	8%					
22	B0	2740	25%	56%	19% •					
23	R0	108	210/	94%	170/					
20		100	71/0	97%	1776					
24	B2	222	44%	52%	•					
25	B3	119	33%	61%	7%					
25	B5	119	34%	96% 59%	7%					
26	BA	227	28%	% 54%	15% ·					
27	BR	209	32%	61%	6% -					
		200	69%	01/0	070 •					
28	BC	198	20%	65% 93%	13% •					
29	BD	177	36%	44%	16% ·					



Mol	Chain	Length	F	Quality of c	hain	
30	BE	167	53%	96%	42%	5%
31	BF	149	64	97% 4%		34% •
32	BG	139	31%	98% 53	%	15% •
33	BH	142	20%	81%		18% 6%
34	BI	122	39% 41%		49%	10%
35	BJ	140	29%	% 40%	_	28% •
36	BK	131	49%		42%	15% •
37	BL	114	29%	71%		18% •
38	BM	113	52%	89%	43%	•
39	BN	114	12%	81% 50%	33	% •
40	BO	115	56% 12%	63%		24% •
41	BQ	106	54%	68%		17%
42	BR	92	15%	58%		23% •
43	BS	99	44%	95%	46%	9%
44	BT	94	48%	94%	47%	5%
45	BU	84	29%	69% 46%		24% •
46	BW	60	27%	78% 60'	%	13%
47	BX	56	39%	95%	57%	
48	BZ	29	21%	100% 45%	2	8% 7%
49	B1	52	35%	96%	5%	17% ·





# 2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 141668 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues		1	AltConf	Trace			
1	AA	1488	Total 31924	C 14238	N 5854	O 10345	Р 1487	0	0

• Molecule 2 is a RNA chain called tRNA.

Mol	Chain	Residues		A	toms		AltConf	Trace		
2 AU	ΔΙΙ	76	Total	С	Ν	0	Р	0	0	
	70	1622	725	293	529	75	0	0		
0		76	Total	С	Ν	0	Р	0	0	
Z AV	70	1622	725	293	529	75	0	0		
2 AW	76	Total	С	Ν	0	Р	0	0		
	AW	AW	AW	70	1622	725	293	529	75	0

• Molecule 3 is a protein called 30S ribosomal subunit protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	236	Total 1847	C 1165	N 328	0 346	S 8	0	0

• Molecule 4 is a protein called 30S ribosomal subunit protein S3.

Mol	Chain	Residues		At	AltConf	Trace			
4	AC	206	Total 1625	C 1028	N 305	O 289	${ m S} { m 3}$	0	0

• Molecule 5 is a protein called 30S ribosomal subunit protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AD	204	Total 1638	C 1023	N 314	O 297	$\frac{S}{4}$	0	0

• Molecule 6 is a protein called 30S ribosomal subunit protein S5.



Mol	Chain	Residues		At	oms	AltConf	Trace		
6	AE	148	Total 1093	C 679	N 208	O 200	S 6	0	0

• Molecule 7 is a protein called 30S ribosomal subunit protein S6.

Mol	Chain	Residues		At	oms		AltConf	Trace	
7	AF	95	Total 784	C 495	N 143	0 140	S 6	0	0

• Molecule 8 is a protein called 30S ribosomal subunit protein S7.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	AG	137	Total 1079	C 671	N 204	O 200	$\frac{S}{4}$	0	0

• Molecule 9 is a protein called 30S ribosomal subunit protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AH	127	Total 968	C 610	N 171	0 181	S 6	0	0

• Molecule 10 is a protein called 30S ribosomal subunit protein S9.

Mol	Chain	Residues		At	oms		AltConf	Trace	
10	AI	126	Total 1014	C 630	N 204	0 177	${ m S} { m 3}$	0	0

• Molecule 11 is a protein called 30S ribosomal subunit protein S10.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	AJ	96	Total 773	C 484	N 148	0 140	S 1	0	0

• Molecule 12 is a protein called 30S ribosomal subunit protein S11.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	AK	116	Total 870	C 535	N 173	0 159	${ m S} { m 3}$	0	0

• Molecule 13 is a protein called 30S ribosomal subunit protein S12.



Mol	Chain	Residues		At	oms			AltConf	Trace
13	AL	101	Total 787	C 486	N 159	O 138	$\frac{S}{4}$	0	0

• Molecule 14 is a protein called 30S ribosomal subunit protein S13.

Mol	Chain	Residues		At	oms			AltConf	Trace
14	AM	115	Total 892	C 552	N 179	0 158	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called 30S ribosomal subunit protein S14.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
15	AN	61	Total 500	C 310	N 108	O 80	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 16 is a protein called 30S ribosomal subunit protein S15.

Mol	Chain	Residues		At	oms			AltConf	Trace
16	AO	86	Total 697	C 430	N 139	0 127	S 1	0	0

• Molecule 17 is a protein called 30S ribosomal subunit protein S16.

Mol	Chain	Residues		At	oms		AltConf	Trace	
17	AP	78	Total 622	C 390	N 122	0 109	S 1	0	0

• Molecule 18 is a protein called 30S ribosomal subunit protein S17.

Mol	Chain	Residues		At	oms			AltConf	Trace
18	AQ	79	Total 640	C 405	N 119	0 113	${ m S} { m 3}$	0	0

• Molecule 19 is a protein called 30S ribosomal subunit protein S18.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	AR	69	Total 576	C 362	N 112	0 101	S 1	0	0

• Molecule 20 is a protein called 30S ribosomal subunit protein S19.



Mol	Chain	Residues		At	oms		AltConf	Trace	
20	AS	87	Total 695	C 443	N 132	O 118	${ m S} { m 2}$	0	0

• Molecule 21 is a protein called 30S ribosomal subunit protein S20.

Mol	Chain	Residues		At	oms	AltConf	Trace		
21	AT	83	Total 649	C 401	N 134	0 111	${f S} {f 3}$	0	0

• Molecule 22 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues			Atoms			AltConf	Trace
22	B0	2740	Total 58824	C 26239	N 10826	O 19019	Р 2740	0	0

• Molecule 23 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues		A	AltConf	Trace			
23	B9	108	Total 2310	C 1030	N 423	O 750	Р 107	0	0

• Molecule 24 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	B2	222	Total 1652	C 1031	N 301	0 314	S 6	0	0

• Molecule 25 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	D2	110	Total	С	Ν	0	S	0	0
2.0	D0	119	845	531	137	174	3	0	0
25	D2	110	Total	С	Ν	0	S	0	0
2.0	D0	119	845	531	137	174	3	0	0

• Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
26	ВА	227	Total 1733	C 1064	N 352	0 311	S 6	0	0

• Molecule 27 is a protein called 50S ribosomal protein L3.



Mol	Chain	Residues		At	oms			AltConf	Trace
27	BB	209	Total 1565	C 979	N 288	O 294	$\frac{S}{4}$	0	0

• Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BC	198	Total 1531	C 960	N 280	0 287	$\begin{array}{c} \mathrm{S} \\ \mathrm{4} \end{array}$	0	0

• Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	BD	177	Total 1415	C 902	N 250	0 257	S 6	0	0

• Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms			AltConf	Trace
30	BE	167	Total 1253	C 789	N 228	0 234	${ m S} { m 2}$	0	0

• Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
21	BE	140	Total	С	Ν	Ο	S	0	0
01	DI	145	1111	699	197	214	1	0	0

• Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
32	BG	139	Total 1019	С 644	N 177	0 192	S 6	0	0

• Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
33	BH	142	Total 1129	C 714	N 212	0 199	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 34 is a protein called 50S ribosomal protein L14.



Mol	Chain	Residues		At	oms			AltConf	Trace
34	BI	122	Total 939	C 588	N 180	O 166	${f S}{5}$	0	0

• Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
35	BJ	140	Total 1017	C 632	N 200	0 184	S 1	0	0

• Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	BK	131	Total 1036	C 661	N 200	0 171	${S \atop 4}$	0	0

• Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	114	Total 908	С 564	N 184	0 156	$\frac{S}{4}$	0	0

• Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
38	BM	113	Total 864	C 534	N 174	O 156	0	0

• Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	BN	114	Total 917	С 574	N 179	0 163	S 1	0	0

• Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
40	BO	115	Total 937	C 598	N 190	O 149	0	0

• Molecule 41 is a protein called 50S ribosomal protein L22.



Mol	Chain	Residues		At	oms			AltConf	Trace
41	BQ	106	Total 825	C 512	N 162	0 149	${ m S} { m 2}$	0	0

• Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		At	oms	AltConf	Trace		
42	BR	92	Total 717	C 455	N 132	O 129	S 1	0	0

• Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		Ato	$\mathbf{ms}$		AltConf	Trace
43	BS	99	Total 762	C 480	N 143	O 139	0	0

• Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		At	oms			AltConf	Trace
44	BT	94	Total 753	C 479	N 137	0 134	${ m S} { m 3}$	0	0

• Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	oms			AltConf	Trace
45	BU	84	Total 634	C 391	N 129	0 113	S 1	0	0

• Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			AltConf	Trace
46	BW	60	Total	С	Ν	Ο	$\mathbf{S}$	0	0
40	DW	00	495	305	96	92	2	0	0

• Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			AltConf	Trace
47	BX	56	Total 435	C 272	N 84	O 77	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 48 is a protein called 50S ribosomal protein L32.



Mol	Chain	Residues		Aton	ıs		AltConf	Trace
48	ΒZ	29	Total 234	C 145	N 47	O 42	0	0

 $\bullet\,$  Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
49	B1	52	Total 424	C 272	N 78	О 74	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S ribosomal RNA











![](_page_15_Figure_3.jpeg)

![](_page_16_Figure_3.jpeg)

![](_page_16_Picture_4.jpeg)

• Molecule 10: 30S ribosomal subunit protein S9

79% Chain AI: 30% 61% 8% •

![](_page_17_Figure_3.jpeg)

![](_page_17_Picture_4.jpeg)

![](_page_18_Figure_3.jpeg)

![](_page_19_Figure_3.jpeg)

![](_page_19_Picture_4.jpeg)

• Molecule 20: 30S ribosomal subunit protein S19

![](_page_19_Figure_6.jpeg)

# V61 162 263 864 965 644 965 647 671 671 671 671 671 671 671 671 671 671 671 673 671 671 671 671 671 771 773 774 774 775 775 776 777 776 777 776 777 776 777 776 777 776 777 776 777 776 777 776 777 776 777

• Molecule 21: 30S ribosomal subunit protein S20

![](_page_19_Figure_9.jpeg)

#### 

![](_page_19_Figure_11.jpeg)

![](_page_20_Figure_3.jpeg)

![](_page_20_Picture_4.jpeg)

G1220	C1221	01222 G1223	U1224	G1225 A1226	G1227	G1228	A1230	U1231	G1232	C1233	G1235	G1236	G1238	G1 239	U1240	A1241	01242 C1243	A1244	G1245	A1246 A1247	G1248	G1250	C1251 G1252	A1253	N1 255	G1256 C1257	U1258 C1259	A1260	C1261 A1262	U1263 A1264	A1265	U1267	A1268 A1269	C1270 G1271	A1272	01273 A1274	A1275 A1276	G1277	C1278 G1279					
G1280	G1281 U1282	G1283 A1284	A1285	A1286	G1288	C1289 C1290	61291	C1293	01294 C1295	G1296	C1297	C1298	G1300	A1301	A1302		C1306	G1310	G1311 U1312	U1313	C1314 C1315	U1316 G1317	U1318		A1321	A1322 C1323	G1324 U1325	U1326	A132/ A1328	01329	G1331	G1333	G1334	G1 <mark>338</mark> G1339	U1340	G1341 A1342	G1343	U1344						
C1345 C1346	A1347	C1351	U1352	G1355	G1355 C1357	G1358 A1359	G1360 G1361	2 2 2 2 2 2	61 364 A1 365	A1366 A1367	G1368	G1369 C1370	<mark>G1371</mark>	U1372	61374	U1375	C1376		61380 61380	G1382	A1383 A1384	A1385	C1386	61388	G1 389	U1390		A1395	U1397	C1398	U1400	G1401	01402 A1403	C1404	U1405	01406 61407	G1408	U1409	G1410	11110				
G1412	U1413	G1414 G1415	G1416	01417 01418	A1419 U1420	G1421 G1422	A1423	G1424 G1425	G1426	A1427	G1429	61430 A1431	G1432	A1433 A1434	G1435	G1 437	U1438	A1439	U1440 G1441	U1442	U1443	A1444	01443 G1446	C1 44 7	C1448	A1449 A1450	G1451	C1452	01453	U1455	G1456	C1458	U1459	G1460	01462	G1463	G1464	01465	G1467	G1468	01469	C1471		
G1472	C1473	01474 C1475	A1476	61478	G1479 G1480	C1481	G1482	U1484	C1485	G1486	G1487	01400 U1489	C1490	A1491	61492 A1403	A1494	A1495	A1496	U1497	C1498 U1499	A1500		G1503	G1504	01505 C1506	A1507	C1508	A1509	G1511	C1512	C1513 U1514	C1515	<b>d1516</b>	A1518	C1519	G1520	01521 A1522	U1523	C1524	G1526	G1527	G1529	C1530	U1531
U1532	C1533	C1536 C1537	G1538	A1539 A1540	G1541	C1542 G1543	A1544	A1545	G1546	A1548	A1549	C1550		A1553	G1555	<mark>U1559</mark>	C1561 U1562	U1563	C1564	A1566	G1567	G1568 A1569	A1570 A1571	A1572	G1573 C1574	U1575 111 576		U1578	A1579	A1581	C1582	01584	U1585	G1586	A158/ A1588	A1589	C1590	U1592	G1593	U1594	C1595 A1596			
A1597	A1598	01599 C1600	G1601 U1602	A1603 C1604	C1605 C1606	C1607 A1608	A1609	A1610 C1611	C1612	A1614	C1615	A1616 C1617	A1618	CTOTE	G1623	A1626	G1627	01629	A1630	A1632	G1633	A1034 A1635	U1636 A1637	C1638	C1039 A1640	G1642 G1643	C1644	C1646	U1647 U1648	G1649 A1650	G1651	G1653	A1654 A1655	C1656 111657	C1658	G1660 G1660								
G1661 111662	G1663	A1664 A1665	G1666 G1667	A1668 A1669	C1670	A1672	G1674 G1674	C1675 A1676	A1677	A1678 A1679	U1680	G1682	U1683 G1684		G1687	U1688	A1690	C1691	U1692	C1694	G1695	G1697	A1698	A1700	A1701 G1702	G1703		C1706	G1707 C1708	U1709		U1712	U1716	G1718	C1728	U1729	C1730	C1732	C1741					
U1742	G1743		C1748	G1750	U1751	C1752	A1755 G1756	A1757	01758 A1759	C1760 C1761	A1762	G1763 C1764	U1765	G1767 G1767	C1768	61770 G1770	C1771 A1773	A1773	C1774 111775	G1776	U1779	A1780 II1781	01781 U1782	A1783 A1784	A1785 A1786	A1787	C1788 A1789	C1790		A1794 C1795	U1796 G1797	U1798 G1799	C1800	A1 80 1 A1 80 2	A1803 C1804	A1805	-							
A1810	G1811 U1812	G1813 G1814	A1815	C1816 G1817	U1818 A1819	U1820 A1821	C1822	G1824	U1825 G1826	U1827	G1828 A1829	C1830	C1832	C1833 U1834	G1835	C1836 C1837	C1838	G1839	G1840 U1841	50 T	C1844 G1845	G1846	A184/ A1848	G1849	G1850	A1853	A1854	01859 G1860		C1870	A1871 A1872	A1877		C1881 U1882	C1887 G1888	A1889	A1890 G1891							
C1892	C1894	C1895 G1896	G1897 111898	A1899	A1900 A1901	C1902 G1903	G1904	C1909	G1910	01911 A1912	A1913	C1914	U1917	A1919	C1920 C1921	G1922	U1923 C1924	C1925	01926	A1928	G1929 G1930	U1931	61933	C1934	G1935 A1936	A1937 A1938	U1939	U1940 C1941	C1942 11643	U1944	01946	C1947 G1948	G1949	A1953	G1954 U1955	U1956	C1957							
C1958 C1958	A1960	C1961 C1962	01963 01964	C1965 A1966	C1967	A1969	01971 U1971	G1972 G1973	C1974	61975 U1976	A1977	G1980	A1981 11982		C1985 C1986	A1987	G1988	G1989	U1991	G1992 U1993	C1994	01995 C1996	C1997 A1998	C1999	C2000 C2001	G2002 A2003	G2004	A2005 C2006	U2007 C2008	A2009	G2010	G2012 A2013	A2014	A2015 U2016	42020	C2021								
U2022 C2023	G2024	C2025	A2030 A2031	G2 032 A 2 033	U2034	C2036	62038	U2039 G2040	U2041	A2042 C2043	C2044	C2045	C2047	G2048 G2049	C2050	A2051 A2052	G2053	A2054 C2055	G2056	G2057 A2058	A2059 A2060	G2061	A2062 C2063	C2064 C2065	C2066	G2067 U2068	G2069 A2070	A2071	C2072 C2073	U2074 U2075	U2076	AZU//	U2086 G2087	A2088	C2089	A2090 C2091								

WORLDWIDE PROTEIN DATA BANK

![](_page_22_Figure_3.jpeg)

A2902

![](_page_22_Picture_5.jpeg)

![](_page_23_Figure_3.jpeg)

 $\bullet$  Molecule 26: 50S ribosomal protein L2

![](_page_24_Figure_4.jpeg)

![](_page_24_Picture_5.jpeg)

# F124 V126 V126 E127 A128 F131 F132 F133 F134 F135 F133 F134 F135 F134 F135 F135 F134 F135 F135 F136 F135 F144 F145 F146 F145 F146 F146 F146 F145 F146

#### D184 K185 V186 V187 M188 M188 A194 A195 A196 A

• Molecule 29: 50S ribosomal protein L5

![](_page_25_Figure_6.jpeg)

 $\bullet$  Molecule 30: 50S ribosomal protein L6

![](_page_25_Figure_8.jpeg)

![](_page_26_Figure_3.jpeg)

![](_page_26_Picture_4.jpeg)

![](_page_27_Figure_3.jpeg)

 $\bullet$  Molecule 36: 50S ribosomal protein L16

![](_page_27_Figure_6.jpeg)

• Molecule 38: 50S ribosomal protein L18

![](_page_27_Figure_8.jpeg)

 $\bullet$  Molecule 39: 50S ribosomal protein L19

![](_page_27_Figure_10.jpeg)

![](_page_27_Picture_11.jpeg)

![](_page_28_Figure_3.jpeg)

![](_page_29_Figure_3.jpeg)

![](_page_29_Picture_4.jpeg)

# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53325	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	CTF correction of 3D-maps by Wiener filtra-	Depositor
	tion	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	11	Depositor
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	4.3	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	454.815	Depositor
Minimum map value	-299.714	Depositor
Average map value	5.836	Depositor
Map value standard deviation	33.806	Depositor
Recommended contour level	46.1	Depositor
Map size (Å)	341.22, 341.22, 341.22	wwPDB
Map dimensions	121, 121, 121	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.82, 2.82, 2.82	Depositor

![](_page_30_Picture_5.jpeg)

# 5 Model quality (i)

#### 5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	B	ond lengths	I	Bond angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	AA	0.67	96/35745~(0.3%)	0.93	170/55764~(0.3%)
2	AU	0.17	0/1814	0.65	0/2827
2	AV	0.17	0/1814	0.64	0/2827
2	AW	0.18	0/1814	0.63	0/2827
3	AB	0.25	0/1877	0.40	0/2523
4	AC	0.23	0/1652	0.42	0/2225
5	AD	0.22	0/1660	0.40	0/2220
6	AE	0.23	0/1106	0.42	0/1488
7	AF	0.24	0/802	0.45	0/1081
8	AG	0.23	0/1093	0.42	0/1467
9	AH	0.23	0/978	0.43	0/1311
10	AI	0.24	0/1026	0.44	0/1364
11	AJ	0.23	0/783	0.46	0/1058
12	AK	0.24	0/886	0.44	0/1195
13	AL	0.22	0/799	0.44	0/1070
14	AM	0.21	0/900	0.43	0/1201
15	AN	0.25	0/510	0.39	0/679
16	AO	0.23	0/705	0.42	0/942
17	AP	0.26	0/632	0.44	0/848
18	AQ	0.24	0/649	0.45	0/870
19	AR	0.25	0/585	0.39	0/782
20	AS	0.25	0/712	0.46	0/955
21	AT	0.24	0/655	0.38	0/866
22	B0	0.40	23/65882~(0.0%)	0.67	20/102783~(0.0%)
23	B9	0.20	0/2583	0.64	0/4028
24	B2	0.22	0/1665	0.44	0/2240
25	B3	0.22	0/842	0.43	0/1123
25	B5	0.22	0/844	0.46	0/1129
26	BA	0.72	$\overline{4/1758}~(0.2\%)$	0.65	$\overline{2/2353}~(0.1\%)$
27	BB	0.56	1/1582~(0.1%)	0.61	1/2122~(0.0%)
28	BC	0.25	0/1549	0.52	0/2082
29	BD	0.26	6 0/1438		0/1927
30	BE	0.23	23 0/1273 0		0/1725
31	BF	0.24	0/1120	0.43	0/1509

![](_page_31_Picture_7.jpeg)

Mal	Chain	E	Bond lengths	I	Bond angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
32	BG	0.25	0/1032	0.54	0/1388
33	BH	0.27	0/1152	0.62	1/1551~(0.1%)
34	BI	0.23	0/948	0.45	0/1269
35	BJ	0.25	0/1025	0.56	0/1363
36	BK	0.27	0/1055	0.48	0/1409
37	BL	0.26	0/920	0.61	0/1229
38	BM	0.22	0/873	0.40	0/1170
39	BN	0.25	0/929	0.51	0/1242
40	BO	1.30	6/949~(0.6%)	3.57	8/1261~(0.6%)
41	BQ	0.23	0/832	0.58	0/1113
42	BR	0.24	0/720	0.54	0/956
43	BS	0.25	0/769	0.42	0/1023
44	BT	0.25	0/766	0.41	0/1025
45	BU	0.27	0/642	0.50	0/848
46	BW	0.24	0/496	0.50	0/658
47	BX	0.23	0/439	0.45	0/587
48	BZ	0.24	0/238	0.45	0/316
49	B1	0.27	0/431	0.46	0/572
All	All	0.46	130/153949~(0.1%)	0.75	202/230391~(0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	1	3
22	B0	5	4
All	All	6	7

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
22	B0	1996	С	N1-C2	33.93	1.74	1.40
22	B0	1579	A	N1-C2	27.63	1.59	1.34
22	B0	1421	G	N1-C2	25.25	1.57	1.37
1	AA	545	С	O3'-P	24.31	1.90	1.61
1	AA	536	С	N1-C6	24.27	1.51	1.37

The worst 5 of 202 bond angle outliers are listed below:

![](_page_32_Picture_9.jpeg)

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
40	BO	100	PHE	CZ-CE2-CD2	-69.61	36.57	120.10
40	BO	100	PHE	CD1-CE1-CZ	-69.56	36.62	120.10
40	BO	100	PHE	CE1-CZ-CE2	-53.35	23.98	120.00
40	BO	100	PHE	CG-CD1-CE1	-32.88	84.64	120.80
40	BO	100	PHE	CG-CD2-CE2	-32.87	84.64	120.80

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	428	G	C1'
22	B0	1593	G	C1'
22	B0	1653	G	C1'
22	B0	2143	С	C1'
22	B0	2250	G	C1'

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	538	G	Sidechain
1	AA	540	G	Sidechain
1	AA	541	G	Sidechain
22	B0	1418	G	Sidechain
22	B0	1579	A	Sidechain

#### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	31924	0	16066	1600	0
2	AU	1622	0	821	102	0
2	AV	1622	0	821	75	0
2	AW	1622	0	821	80	0
3	AB	1847	0	1855	120	0
4	AC	1625	0	1699	164	0
5	AD	1638	0	1702	185	0
6	AE	1093	0	1132	117	0
7	AF	784	0	776	100	0
8	AG	1079	0	1108	91	0

![](_page_33_Picture_12.jpeg)

Conti	nuea fron	<i>i previous</i>	page			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AH	968	0	1021	96	0
10	AI	1014	0	1064	153	0
11	AJ	773	0	812	71	0
12	AK	870	0	878	98	0
13	AL	787	0	825	81	0
14	AM	892	0	954	65	0
15	AN	500	0	526	51	0
16	AO	697	0	716	72	0
17	AP	622	0	637	77	0
18	AQ	640	0	678	49	0
19	AR	576	0	599	55	0
20	AS	695	0	725	118	0
21	AT	649	0	697	67	0
22	B0	58824	0	29589	3943	0
23	B9	2310	0	1173	79	0
24	B2	1652	0	1730	181	0
25	B3	845	0	876	139	0
25	B5	845	0	878	133	0
26	BA	1733	0	1764	643	0
27	BB	1565	0	1612	264	0
28	BC	1531	0	1593	499	0
29	BD	1415	0	1451	166	0
30	BE	1253	0	1289	87	0
31	BF	1111	0	1146	48	0
32	BG	1019	0	1076	134	0
33	BH	1129	0	1162	273	0
34	BI	939	0	1011	95	0
35	BJ	1017	0	1086	283	0
36	BK	1036	0	1109	154	0
37	BL	908	0	946	174	0
38	BM	864	0	902	60	0
39	BN	917	0	965	236	0
40	BO	937	0	1008	249	0
41	BQ	825	0	886	220	0
42	BR	717	0	770	187	0
43	BS	762	0	809	72	0
44	BT	753	0	780	45	0
45	BU	634	0	656	172	0
46	BW	495	0	530	76	0
47	BX	435	0	470	41	0
48	BZ	234	0	235	43	0
49	B1	424	0	461	68	0

 $\alpha$ ntia J fa

![](_page_34_Picture_6.jpeg)

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	141668	0	94896	10859	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

The worst 5 of 10859 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B0:1579:A:C2	26:BA:67:LYS:CA	1.76	1.66
22:B0:1996:C:C2	27:BB:138:LEU:CA	1.77	1.62
22:B0:1579:A:C4	26:BA:67:LYS:CA	1.86	1.52
22:B0:1579:A:C4	26:BA:67:LYS:HA	1.38	1.52
22:B0:1421:G:N1	26:BA:149:LYS:CA	1.71	1.51

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	AB	230/236~(98%)	193 (84%)	28 (12%)	9 (4%)	3 23
4	AC	204/206~(99%)	160 (78%)	34 (17%)	10 (5%)	2 20
5	AD	202/204~(99%)	177 (88%)	22 (11%)	3 (2%)	10 46
6	AE	146/148~(99%)	135 (92%)	10 (7%)	1 (1%)	22 63
7	AF	93/95~(98%)	81 (87%)	10 (11%)	2 (2%)	6 35
8	AG	135/137~(98%)	114 (84%)	13 (10%)	8 (6%)	1 17
9	AH	125/127~(98%)	113 (90%)	9 (7%)	3 (2%)	6 33
10	AI	124/126~(98%)	93 (75%)	20 (16%)	11 (9%)	1 11
11	AJ	94/96~(98%)	73 (78%)	15 (16%)	6 (6%)	1 16

![](_page_35_Picture_15.jpeg)

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	entiles
12	AK	114/116~(98%)	91 (80%)	14~(12%)	9~(8%)	1	13
13	AL	99/101~(98%)	75~(76%)	19~(19%)	5 (5%)	2	19
14	AM	111/115~(96%)	90 (81%)	18~(16%)	3~(3%)	5	31
15	AN	59/61~(97%)	50~(85%)	5 (8%)	4 (7%)	1	15
16	AO	84/86~(98%)	76 (90%)	8 (10%)	0	100	100
17	AP	76/78~(97%)	62 (82%)	13 (17%)	1 (1%)	12	48
18	AQ	77/79~(98%)	65~(84%)	10 (13%)	2(3%)	5	31
19	AR	67/69~(97%)	62 (92%)	5 (8%)	0	100	100
20	AS	85/87~(98%)	69~(81%)	12 (14%)	4(5%)	2	21
21	AT	81/83~(98%)	68 (84%)	11 (14%)	2(2%)	5	32
24	B2	216/222~(97%)	183 (85%)	27~(12%)	6 (3%)	5	30
25	B3	108/119~(91%)	84 (78%)	18 (17%)	6 (6%)	2	19
25	B5	112/119~(94%)	89~(80%)	16 (14%)	7~(6%)	1	17
26	BA	215/227~(95%)	128 (60%)	56~(26%)	31 (14%)	0	4
27	BB	199/209~(95%)	148 (74%)	37~(19%)	14 (7%)	1	14
28	BC	194/198~(98%)	124 (64%)	45~(23%)	25~(13%)	0	5
29	BD	173/177~(98%)	96~(56%)	54 (31%)	23~(13%)	0	5
30	BE	165/167~(99%)	141 (86%)	22~(13%)	2(1%)	13	50
31	$_{\mathrm{BF}}$	143/149~(96%)	121 (85%)	16 (11%)	6 (4%)	3	22
32	BG	135/139~(97%)	85~(63%)	33~(24%)	17 (13%)	0	5
33	BH	140/142~(99%)	77~(55%)	41 (29%)	22 (16%)	0	3
34	BI	120/122~(98%)	93~(78%)	20~(17%)	7~(6%)	1	18
35	BJ	136/140~(97%)	69~(51%)	37~(27%)	30 (22%)	0	1
36	BK	129/131~(98%)	93~(72%)	24 (19%)	12 (9%)	0	11
37	BL	110/114~(96%)	67~(61%)	32~(29%)	11 (10%)	0	9
38	BM	111/113~(98%)	90 (81%)	16 (14%)	5 (4%)	2	22
39	BN	112/114~(98%)	50~(45%)	35~(31%)	27 (24%)	0	1
40	BO	$111/115~(\overline{96\%})$	59~(53%)	39~(35%)	13 (12%)	0	6
41	BQ	104/106~(98%)	68~(65%)	29 (28%)	7 (7%)	1	15
42	BR	83/92 (90%)	39~(47%)	25 (30%)	19 (23%)	0	1
43	BS	$95/\overline{99}~(96\%)$	69(73%)	21 (22%)	5 (5%)	2	19

![](_page_36_Picture_6.jpeg)

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
44	BT	92/94~(98%)	76 (83%)	13 (14%)	3 (3%)	4	26
45	BU	82/84~(98%)	43 (52%)	23 (28%)	16 (20%)	0	2
46	BW	58/60~(97%)	49 (84%)	5(9%)	4 (7%)	1	15
47	BX	54/56~(96%)	51 (94%)	3 (6%)	0	100	100
48	BZ	27/29~(93%)	11 (41%)	6 (22%)	10 (37%)	0	0
49	B1	50/52~(96%)	27 (54%)	19 (38%)	4 (8%)	1	12
All	All	5480/5639~(97%)	4077 (74%)	988 (18%)	415 (8%)	2	13

5 of 415 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AB	14	HIS
3	AB	93	HIS
4	AC	126	ARG
4	AC	178	ARG
8	AG	31	VAL

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
3	AB	195/195~(100%)	190~(97%)	5 (3%)	46	66
4	AC	170/170~(100%)	164~(96%)	6 (4%)	36	59
5	AD	172/172~(100%)	170~(99%)	2(1%)	71	83
6	AE	112/112~(100%)	108~(96%)	4 (4%)	35	59
7	AF	83/83~(100%)	80~(96%)	3~(4%)	35	59
8	AG	112/112~(100%)	108~(96%)	4 (4%)	35	59
9	AH	103/103~(100%)	100~(97%)	3~(3%)	42	64
10	AI	104/104~(100%)	100~(96%)	4 (4%)	33	57
11	AJ	$8\overline{4/84}~(100\%)$	80~(95%)	4 (5%)	25	51
12	AK	89/89 (100%)	86~(97%)	3~(3%)	37	60

![](_page_37_Picture_12.jpeg)

Continued from	n previous	page
----------------	------------	------

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
13	AL	85/85~(100%)	82~(96%)	3~(4%)	36	59
14	AM	93/93~(100%)	90~(97%)	3~(3%)	39	61
15	AN	52/52~(100%)	51 (98%)	1 (2%)	57	75
16	AO	74/74~(100%)	74 (100%)	0	100	100
17	AP	63/63~(100%)	60~(95%)	3~(5%)	25	51
18	AQ	73/73~(100%)	72~(99%)	1 (1%)	67	80
19	AR	60/60~(100%)	59~(98%)	1 (2%)	60	78
20	AS	75/75~(100%)	73~(97%)	2(3%)	44	65
21	AT	63/63~(100%)	56~(89%)	7 (11%)	6	22
24	B2	172/172~(100%)	166 (96%)	6 (4%)	36	59
25	B3	83/83~(100%)	81 (98%)	2(2%)	49	69
25	B5	83/83~(100%)	80 (96%)	3 (4%)	35	59
26	BA	176/176~(100%)	159 (90%)	17 (10%)	8	27
27	BB	164/164~(100%)	160 (98%)	4 (2%)	49	69
28	BC	163/163~(100%)	152 (93%)	11 (7%)	16	41
29	BD	149/149~(100%)	124 (83%)	25 (17%)	2	12
30	BE	130/130~(100%)	123~(95%)	7 (5%)	22	47
31	BF	114/114~(100%)	112 (98%)	2(2%)	59	77
32	BG	108/108~(100%)	91~(84%)	17~(16%)	2	14
33	BH	116/116~(100%)	94 (81%)	22~(19%)	1	8
34	BI	103/103~(100%)	97~(94%)	6 (6%)	20	45
35	BJ	99/99~(100%)	74 (75%)	25 (25%)	0	3
36	BK	104/104~(100%)	90 (86%)	14 (14%)	4	17
37	BL	94/94~(100%)	80 (85%)	14 (15%)	3	15
38	BM	83/83~(100%)	78~(94%)	5~(6%)	19	44
39	BN	99/99~(100%)	74 (75%)	25 (25%)	0	3
40	BO	89/89~(100%)	70 (79%)	19 (21%)	1	6
41	BQ	89/89~(100%)	76~(85%)	13 (15%)	3	15
42	BR	77/77~(100%)	65 (84%)	12 (16%)	2	14
43	BS	82/82~(100%)	77 (94%)	5 (6%)	18	44
44	BT	78/78~(100%)	75~(96%)	3 (4%)	33	57

![](_page_38_Picture_6.jpeg)

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	BU	62/62~(100%)	52 (84%)	10 (16%)	2 13
46	BW	55/55~(100%)	50 (91%)	5 (9%)	9 29
47	BX	47/47~(100%)	45~(96%)	2(4%)	29 53
48	BZ	24/24~(100%)	18~(75%)	6(25%)	0 3
49	B1	46/46~(100%)	37~(80%)	9(20%)	1 8
All	All	4551/4551~(100%)	4203~(92%)	348 (8%)	17 37

5 of 348 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	BL	75	ILE
41	BQ	18	ARG
38	BM	88	LYS
39	BN	92	ARG
42	BR	64	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such side chains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
40	BO	36	GLN
41	BQ	9	HIS
46	BW	15	ASN
16	AO	34	GLN
16	AO	19	ASN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1487/1488~(99%)	248~(16%)	71 (4%)
2	AU	75/76~(98%)	13 (17%)	5~(6%)
2	AV	75/76~(98%)	10 (13%)	4(5%)
2	AW	75/76~(98%)	13 (17%)	5~(6%)
22	B0	2739/2740 (99%)	541 (19%)	131 (4%)
23	B9	107/108~(99%)	20 (18%)	2(1%)
All	All	4558/4564 (99%)	845 (18%)	218 (4%)

 $5~{\rm of}~845$  RNA backbone outliers are listed below:

![](_page_39_Picture_12.jpeg)

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	А
1	AA	9	G
1	AA	13	U
1	AA	31	G

5 of 218 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	B0	784	G
22	B0	1302	А
22	B0	2433	А
22	B0	846	U
22	B0	1061	U

#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	B3	6
26	BA	5
25	B5	4

![](_page_40_Picture_18.jpeg)

Mol	Chain	Number of breaks
27	BB	4
42	BR	4
24	B2	2
3	AB	2
31	BF	2
1	AA	2
28	BC	1
29	BD	1
14	AM	1
43	BS	1
32	BG	1
37	BL	1
40	BO	1
35	BJ	1

The worst 5 of 39 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B5	52:THR	С	53:GLU	N	10.02
1	BA	60:ALA	С	61:TYR	N	9.99
1	B5	50:GLU	С	51:LYS	N	9.70
1	BB	167:ASN	С	168:GLU	N	8.31
1	BC	96:VAL	С	97:ASN	N	7.51

![](_page_41_Picture_7.jpeg)

# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1143. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

#### 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map

![](_page_42_Picture_8.jpeg)

The images above show the map projected in three orthogonal directions.

#### 6.2 Central slices (i)

#### 6.2.1 Primary map

![](_page_42_Picture_12.jpeg)

X Index: 60

![](_page_42_Picture_14.jpeg)

Y Index: 60

![](_page_42_Picture_16.jpeg)

Z Index: 60

![](_page_42_Picture_18.jpeg)

The images above show central slices of the map in three orthogonal directions.

#### 6.3 Largest variance slices (i)

#### 6.3.1 Primary map

![](_page_43_Picture_6.jpeg)

X Index: 60

Y Index: 60

Z Index: 55

The images above show the largest variance slices of the map in three orthogonal directions.

#### 6.4 Orthogonal surface views (i)

#### 6.4.1 Primary map

![](_page_43_Picture_13.jpeg)

The images above show the 3D surface view of the map at the recommended contour level 46.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

![](_page_43_Picture_15.jpeg)

### 6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

![](_page_44_Picture_5.jpeg)

# 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

#### 7.1 Map-value distribution (i)

![](_page_45_Figure_6.jpeg)

The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

![](_page_45_Picture_8.jpeg)

#### 7.2 Volume estimate (i)

![](_page_46_Figure_4.jpeg)

The volume at the recommended contour level is 2036  $\rm nm^3;$  this corresponds to an approximate mass of 1839 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

![](_page_46_Picture_7.jpeg)

#### 7.3 Rotationally averaged power spectrum (i)

![](_page_47_Figure_4.jpeg)

\*Reported resolution corresponds to spatial frequency of 0.067  ${\rm \AA^{-1}}$ 

![](_page_47_Picture_6.jpeg)

# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

![](_page_48_Picture_5.jpeg)

## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1143 and PDB model 4V4W. Per-residue inclusion information can be found in section 3 on page 13.

#### 9.1 Map-model overlay (i)

![](_page_49_Picture_6.jpeg)

The images above show the 3D surface view of the map at the recommended contour level 46.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

![](_page_49_Picture_8.jpeg)

#### 9.2 Q-score mapped to coordinate model (i)

![](_page_50_Figure_4.jpeg)

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

#### 9.3 Atom inclusion mapped to coordinate model (i)

![](_page_50_Figure_7.jpeg)

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (46.1).

![](_page_50_Picture_9.jpeg)

#### 9.4 Atom inclusion (i)

![](_page_51_Figure_4.jpeg)

At the recommended contour level, 36% of all backbone atoms, 41% of all non-hydrogen atoms, are inside the map.

![](_page_51_Picture_6.jpeg)

1.0

0.0 <0.0

#### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (46.1) and Q-score for the entire model and for each chain.

All       0.4138       -0.004         AA       0.4810       -0.001         AB       0.0314       -0.007         AC       0.1039       -0.025         AD       0.0095       0.0000         AE       0.1214       0.0140         AF       0.0223       -0.013         AG       0.0755       -0.037         AH       0.0011       -0.013         AI       0.2080       0.0060         AJ       0.2112       0.0220         AK       0.2565       -0.024         AL       0.7141       0.0080         AM       0.1535       0.0250         AN       0.0000       -0.026	
AA       0.4810       -0.001         AB       0.0314       -0.007         AC       0.1039       -0.025         AD       0.0095       0.0000         AE       0.1214       0.0140         AF       0.0223       -0.013         AG       0.0755       -0.037         AH       0.0011       -0.013         AI       0.2080       0.0060         AJ       0.2112       0.0220         AK       0.2565       -0.024         AL       0.7141       0.0080         AM       0.1535       0.0250         AN       0.0000       -0.026	0
AB       0.0314       -0.007         AC       0.1039       -0.025         AD       0.0095       0.000         AE       0.1214       0.014         AF       0.0223       -0.013         AG       0.0755       -0.037         AH       0.0011       -0.013         AI       0.2080       0.0060         AJ       0.2112       0.0220         AK       0.2565       -0.024         AL       0.7141       0.0080         AM       0.1535       0.0250         AN       0.0000       -0.026	0
AC       0.1039       -0.025         AD       0.0095       0.000         AE       0.1214       0.0140         AF       0.0223       -0.013         AG       0.0755       -0.037         AH       0.0011       -0.013         AI       0.2080       0.0060         AJ       0.2112       0.0220         AK       0.2565       -0.024         AL       0.7141       0.0080         AM       0.1535       0.0250         AN       0.0000       -0.026	0
AD       0.0095       0.0000         AE       0.1214       0.014         AF       0.0223       -0.013         AG       0.0755       -0.037         AH       0.0011       -0.013         AI       0.2080       0.0060         AJ       0.2112       0.0220         AK       0.2565       -0.024         AL       0.7141       0.0080         AM       0.1535       0.0250         AN       0.0000       -0.026	0
AE       0.1214       0.0140         AF       0.0223       -0.013         AG       0.0755       -0.037         AH       0.0011       -0.013         AI       0.2080       0.0060         AJ       0.2112       0.0220         AK       0.2565       -0.024         AL       0.7141       0.0080         AM       0.1535       0.0250         AN       0.0000       -0.026	0
AF       0.0223       -0.013         AG       0.0755       -0.037         AH       0.0011       -0.013         AI       0.2080       0.0060         AJ       0.2112       0.0220         AK       0.2565       -0.024         AL       0.7141       0.0080         AM       0.1535       0.0250         AN       0.0000       -0.026	0
AG       0.0755       -0.037         AH       0.0011       -0.013         AI       0.2080       0.0060         AJ       0.2112       0.0220         AK       0.2565       -0.024         AL       0.7141       0.0080         AM       0.1535       0.0250         AN       0.0000       -0.026	0
AH       0.0011       -0.013         AI       0.2080       0.0060         AJ       0.2112       0.0220         AK       0.2565       -0.024         AL       0.7141       0.0080         AM       0.1535       0.0250         AN       0.0000       -0.026         AO       0.2141       0.001	0
AI       0.2080       0.0060         AJ       0.2112       0.0220         AK       0.2565       -0.024         AL       0.7141       0.0080         AM       0.1535       0.0250         AN       0.0000       -0.026         AO       0.2141       0.001	0
AJ     0.2112     0.0220       AK     0.2565     -0.024       AL     0.7141     0.0080       AM     0.1535     0.0250       AN     0.0000     -0.026       AO     0.2141     0.001	0
AK     0.2565     -0.024       AL     0.7141     0.008       AM     0.1535     0.025       AN     0.0000     -0.026       AO     0.3141     0.001	0
AL     0.7141     0.0080       AM     0.1535     0.0250       AN     0.0000     -0.026       AO     0.3141     0.001	0
AM     0.1535     0.0250       AN     0.0000     -0.026       AO     0.3141     0.001	0
AN 0.0000 -0.026	0
	60
AU 0.0141 -0.001	0
AP 0.0117 -0.028	0
AQ 0.1891 0.0050	0
AR 0.2686 -0.011	0
AS 0.0486 0.0110	0
AT 0.2098 -0.015	0
AU 0.5191 0.000	0
AV 0.7417 -0.004	:0
AW 0.6264 0.016	0
B0 0.5457 -0.006	60
B1 0.0264 -0.024	0
B2 0.0289 -0.008	50
B3 0.2218 0.030	0
B5 0.0403 -0.017	0
B9 0.0567 -0.015	0
BA 0.2171 -0.023	0
BB 0.2594 0.008	0
BC 0.3022 0.006	0
BD 0.0588 -0.013	0
BE 0.0553 -0.007	0

![](_page_52_Picture_7.jpeg)

Chain	Atom inclusion	Q-score
BF	0.0283	-0.0110
BG	0.0139	0.0070
BH	0.1573	-0.0050
BI	0.5635	-0.0000
BJ	0.3778	0.0150
BK	0.4910	-0.0190
BL	0.2769	0.0090
BM	0.1030	0.0080
BN	0.1644	-0.0370
BO	0.4276	0.0230
BQ	0.4328	-0.0150
BR	0.4567	0.0160
BS	0.0467	-0.0280
BT	0.0678	0.0110
BU	0.3107	-0.0010
BW	0.1946	0.0080
BX	0.0378	0.0030
BZ	0.0000	-0.0130

![](_page_53_Picture_5.jpeg)